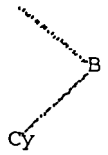
```
=> file casreact
FILE 'CASREACT' ENTERED AT 16:41:10 ON 10 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 5 May 2007 VOL 146 ISS 20

New CAS Information Use Policies, enter HELP USAGETERMS for details.

************************************************************
*                                                          *
*     CASREACT now has more than 12 million reactions      *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> d stat que L8
L3              STR
```

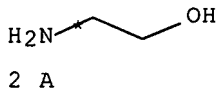



```
Structure attributes must be viewed using STN Express query preparation:
Uploading L3.str

L4         39926 SEA FILE=REGISTRY SSS FUL L3
L5               STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L5.str

L6          3643 SEA FILE=CASREACT ABB=ON  PLU=ON  L4
L8            13 SEA FILE=CASREACT SUB=L6 SSS FUL L5 (    79 REACTIONS)

100.0% DONE      492 VERIFIED      79 HIT RXNS                    13 DOCS
SEARCH TIME: 00.00.01
```

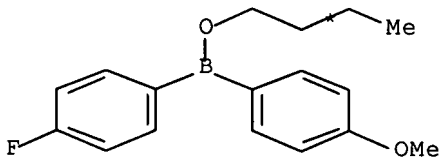
L8 ANSWER 11 OF 13 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 112:139083 CASREACT Full-text
TITLE: Studies on antitumor boron compounds. V. Fluorine- and methoxy-substituted diphenylboron chelates with N,O-bidentate ligands
AUTHOR(S): Yuan, Guozheng; Pang, Jinxin; Zhang, Guomin; Zeng, Fanbo
CORPORATE SOURCE: Dep. Chem., Wuhan Univ., Wuhan, Peop. Rep. China
SOURCE: Youji Huaxue (1989), 9(3), 226-9
CODEN: YCHHDX; ISSN: 0253-2786
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB Title diphenylboron chelates of ethanolamine, 2-amino-1-butanol, dl-norvaline, dl-norleucine, dl-phenylalanine, and 8-hydroxyquinoline were prepared Their antitumor effects on mice were tested.

RX(1) OF 41 ...2 A + 2 ***B*** ===> ***C*** + D

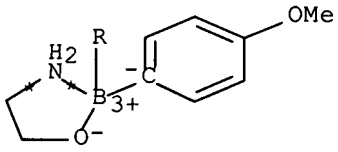


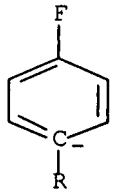
2 A



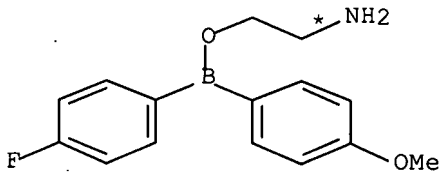
2 B

(1) →



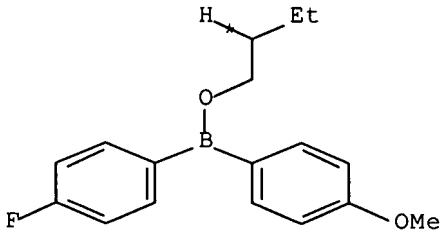


C
YIELD 92%

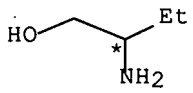


D
YIELD 92%

RX(2) OF 41 ...2 ***B*** + 2 G ===> ***H*** + I

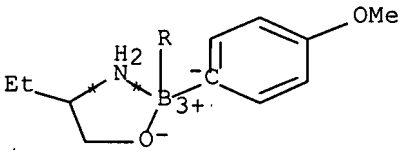


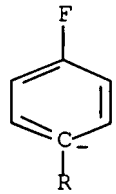
2 B



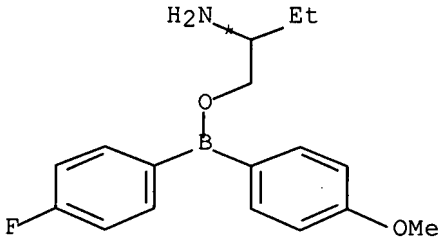
2 G

(2) ⟶



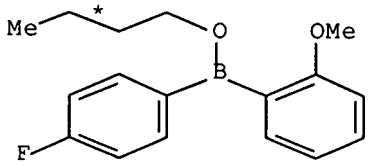


H
YIELD 73%

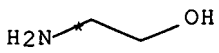


I
YIELD 73%

RX(3) OF 41 ...2 ***J*** + 2 A ===> ***K*** + L

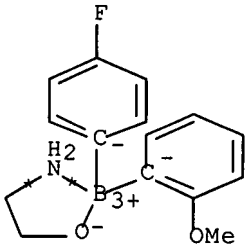


2 J

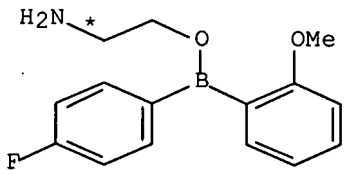


2 A

(3) ⟶



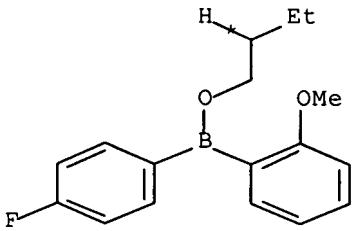
K
YIELD 91%



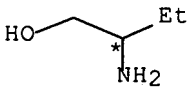
L
YIELD 91%

RX(3) RCT J ***100689-51-8***, A 141-43-5
PRO K ***125842-39-9***, L 125553-29-9
SOL 64-17-5 EtOH, 7732-18-5 Water

RX(4) OF 41 ...2 ***J*** + 2 G ===> ***M*** + N

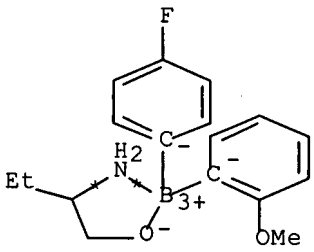


2 J

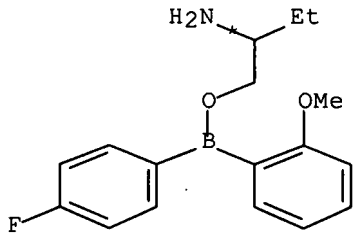


2 G

(4) ⟶

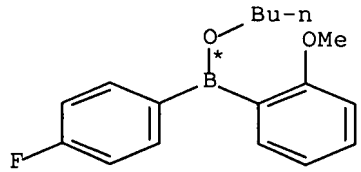


M
YIELD 71%

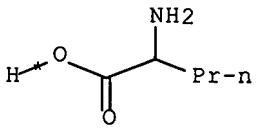


N
YIELD 71%

RX(8) OF 41 ...2 ***J*** + 2 O ===> ***Y*** + Z

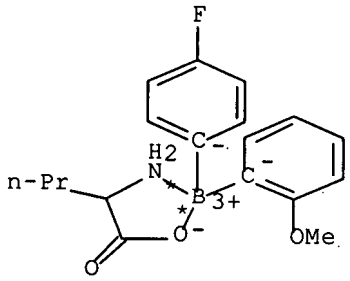


2 J

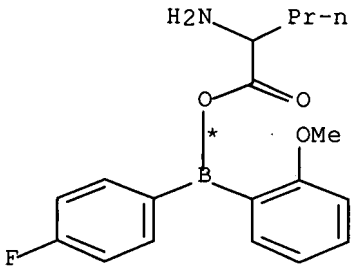


2 O

(8) ⟶



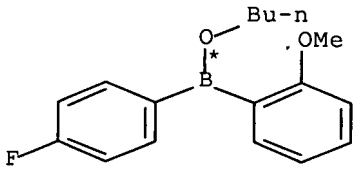
Y
YIELD 95%



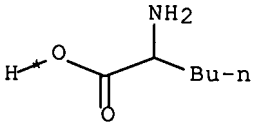
Z
YIELD 95%

RX(8) RCT J ***100689-51-8***, O 760-78-1
PRO Y ***125869-40-1***, Z 125553-34-6
SOL 108-88-3 PhMe

RX(9) OF 41 ...2 ***J*** + 2 S ===> ***AA*** + AB

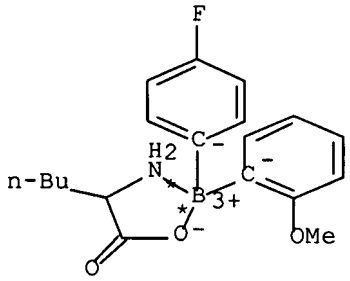


2 J

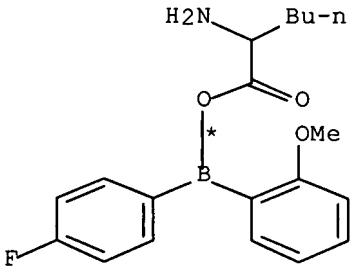


2 S

(9) ⟶



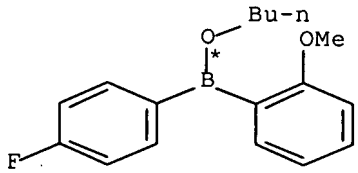
AA
YIELD 76%



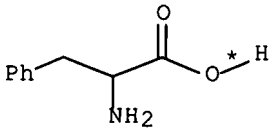
AB
YIELD 76%

RX(9) RCT J ***100689-51-8***, S 616-06-8
PRO AA ***125842-44-6***, AB 125553-35-7
SOL 108-88-3 PhMe

RX(10) OF 41 ...2 ***J*** + 2 V ===> ***AC*** + AD

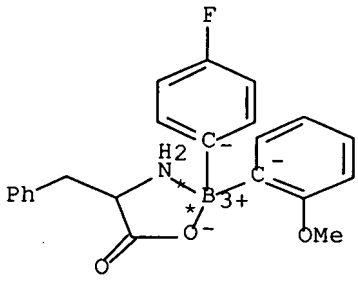


2 J

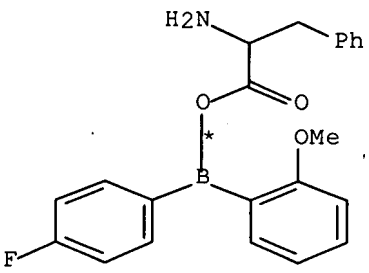


2 V

(10)



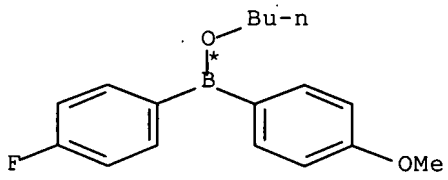
AC
YIELD 63%



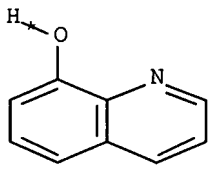
AD
YIELD 63%

RX(10) RCT J ***100689-51-8***, V 150-30-1
PRO AC ***125842-45-7***, AD 125553-36-8
SOL 108-88-3 PhMe

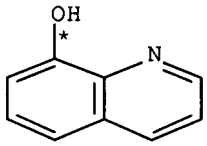
RX(11) OF 41 ...2 ***B*** + 2 AE ===> ***AF*** + AG



2 B

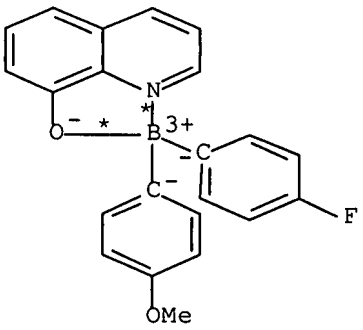


AE

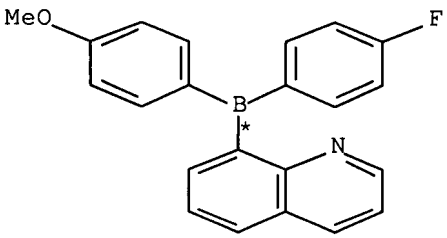


AE

(11)



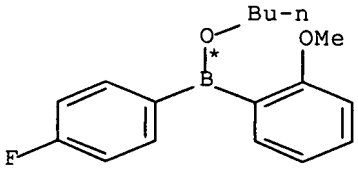
AF
YIELD 95%



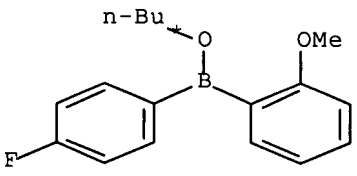
AG
YIELD 95%

RX(11) RCT B ***125553-26-6***, AE 148-24-3
PRO AF ***125842-46-8***, AG 125553-37-9
SOL 64-17-5 EtOH

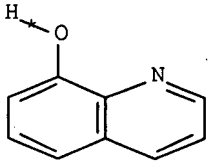
RX(12) OF 41 ...2 ***J*** + 2 AE ===> ***AH*** + AI



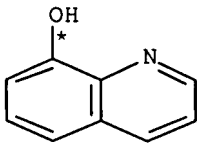
J



J

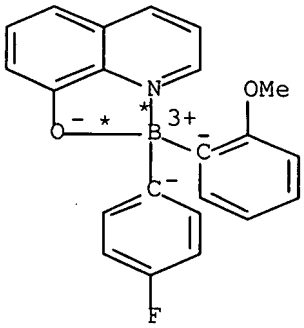


AE

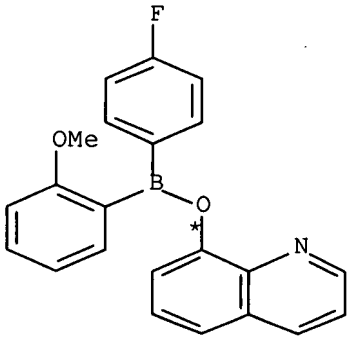


AE

(12)



AH
YIELD 94%



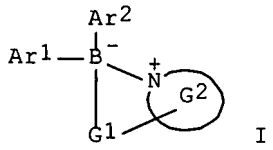
AI
YIELD 94%

RX(12) RCT J ***100689-51-8***, AE 148-24-3
PRO AH ***101754-10-3***, AI 100689-52-9
SOL 64-17-5 EtOH

L16 ANSWER 6 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:535001 CAPLUS Full-text
DOCUMENT NUMBER: 133:144898
TITLE: Organoboron compounds exhibiting anticoccidial activities
INVENTOR(S): Imazaki, Hideyuki; Fujikawa, Masazumi; Hayase, Yoshio; Kawaguchi, Harumoto
PATENT ASSIGNEE(S): Nitto Kasei Co., Ltd., Japan; Shionogi and Co., Ltd.
SOURCE: PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000044387	A1	20000803	WO 1999-JP7139	19991220
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1155698	A1	20011121	EP 1999-959910	19991220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

PRIORITY APPLN. INFO.: JP 1999-21822 A 19990129
WO 1999-JP7139 W 19991220
OTHER SOURCE(S): MARPAT 133:144898
GI

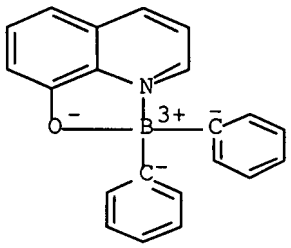


I

AB Drug compns. for animals (except Home sapiens), antiprotozoal agents and anticoccidial agents, containing compds. represented by general formula (I), salts of the same, or hydrates of both, wherein Ar1 and Ar2 are each independently an optionally substituted cyclic group; G1 is -A-, -A-CR1R2-, or -A-CR3R4-CR5R6-; and G2 is an optionally substituted azacyclic group (wherein the ring-constituting nitrogen atom is bonded to B-) or the like, provided the ring composed of B-, G1 and G2 is a five- or six-membered one.

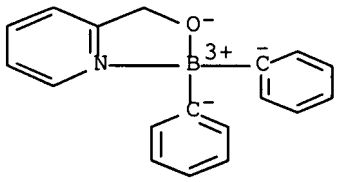
IT ***29190-60-1P 52997-17-8P 132722-17-9P 137001-21-9P 159097-99-1P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(organoboron compds. exhibiting anticoccidial and antiprotozoal activities)

RN 29190-60-1 CAPLUS
CN Boron, diphenyl(8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)



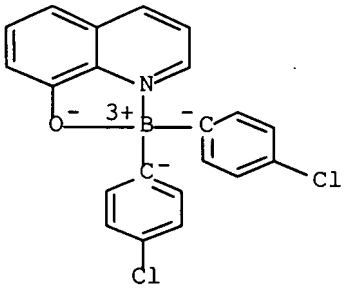
RN 52997-17-8 CAPLUS

CN Boron, diphenyl(2-pyridinemethanolato-κN1,κO2)-, (T-4)- (9CI) (CA INDEX NAME)



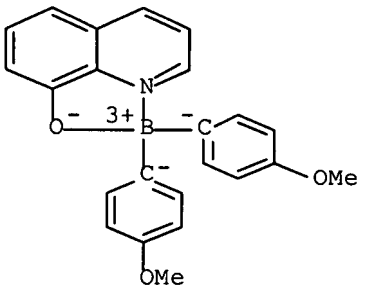
RN 132722-17-9 CAPLUS

CN Boron, bis(4-chlorophenyl)(8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)



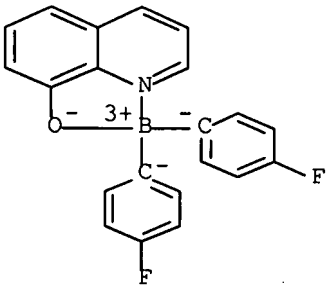
RN 137001-21-9 CAPLUS

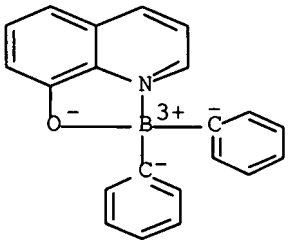
CN Boron, bis(4-methoxyphenyl)(8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)



RN 159097-99-1 CAPLUS

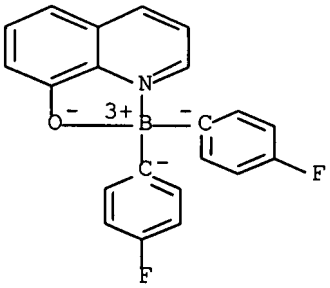
CN Boron, bis(4-fluorophenyl)(8-quinolinolato-κN1,κO8)-, (T-4)-(9CI) (CA INDEX NAME)





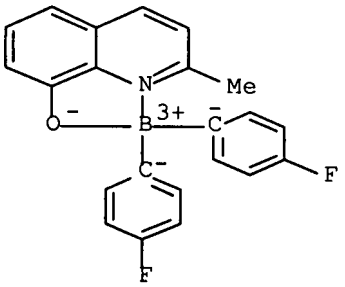
RN 159097-99-1 CAPLUS

CN Boron, bis(4-fluorophenyl)(8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)



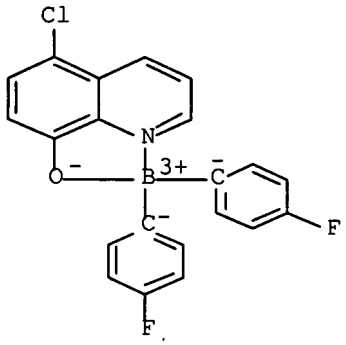
RN 159098-00-7 CAPLUS

CN Boron, bis(4-fluorophenyl)(2-methyl-8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)



RN 159098-01-8 CAPLUS

CN Boron, (5-chloro-8-quinolinolato-κN1,κO8)bis(4-fluorophenyl)-, (T-4)- (9CI) (CA INDEX NAME)

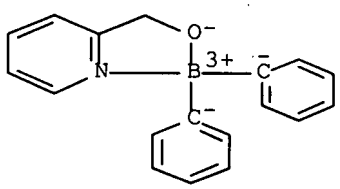

Cl
N
O
-
B
3+
C
-
C
-
F
F

L16 ANSWER 13 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:332485 CAPLUS Full-text
DOCUMENT NUMBER: 120:332485
TITLE: Rotating-bomb combustion calorimetry and the standard enthalpies of formation of two borinic esters
AUTHOR(S): Torres, Luis Alfonso; Perez, Alejandro; Farfan, Norberto; Castillo, Dolores; Santillan, Rosa Luisa
CORPORATE SOURCE: Dep. Quim., Cent. Investigacion, Mexico City, 07000, Mex.
SOURCE: Journal of Chemical Thermodynamics (1994), 26(4), 337-43
CODEN: JCTDAF; ISSN: 0021-9614
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The standard massic energies of combustion of two borinic esters containing the intramol. N → B bond having different stabilities were determined by oxygen rotating-bomb combustion calorimetry. The studied compds. were: diphenyl(2-pyridylmethoxy-O,N)borane (A1) and di-Ph {2-(2'-pyridyl)ethoxy-O,N}borane (A2). Based on the exptl. results, the standard molar enthalpies of formation were determined as : ΔfHmo{C18H16ONB(A1),cr} = -(194.6±4.9)kJ·mol-1 and ΔfHmo{C19H18ONB(A2),cr} = -(171.8±3.2) kJ·mol-1.

IT ***52997-17-8***
RL: PRP (Properties)
(heat of formation of, determination by rotating-bomb combustion calorimetry)

RN 52997-17-8 CAPLUS
CN Boron, diphenyl(2-pyridinemethanolato-κN1,κO2)-, (T-4)- (9CI) (CA INDEX NAME)

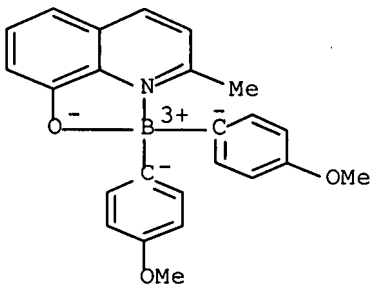


L16 ANSWER 15 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:619486 CAPLUS Full-text
DOCUMENT NUMBER: 115:219486
TITLE: Structure studies of bis(substituted)-2-(substituted)-8-hydroxyquinolines
AUTHOR(S): Liu, Xiaolan; Zhang, Xin; Miao, Fangming; Zhang, Shaohui; Lin, Kai; Zhang, Guomin; Han, Yuzhen; Xu, Xiaojie
CORPORATE SOURCE: Dep. Chem., Tianjin Normal Univ., Tianjin, 300074, Peop. Rep. China
SOURCE: Youji Huaxue (1991), 11(4), 410-15
CODEN: YCHHDX; ISSN: 0253-2786
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

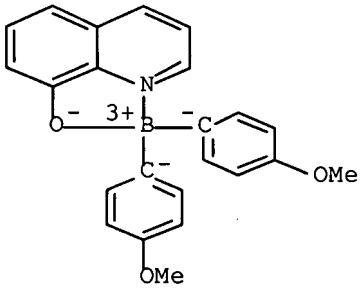
AB Bis(p-methoxyphenyl)-2-methyl-8-hydroxyquinoline borolactone (I) is orthorhombic, space group Pbca, with a 1.1741(5), b 1.6104(3), and c 2.1066(5) nm; Z = 8, R = 0.043. Bis(p-methoxyphenyl)-8-hydroxyquinoline borolactone (II) is monoclinic, space group P21/a, and a 1.0008(1), b 1.3956(2), c 1.3617(3)nm, and β 100.15(1)°; Z = 4, R = 0.089. The structures of the 2 compds. were solved by direct method. The atoms of B, C(39), C(37), N and O(3) form a chelate ring with coordinated bond between B and N atoms. Dihedral angle between two benzenes is 57.8° for I and 95.7° for II. The bond order and charge d. from quantum chemical calcn. indicate the covalent nature of the bonds involving B atom. Atomic coordinates are given.

IT ***137001-20-8 137001-21-9***
RL: PRP (Properties)
(crystal structure of)

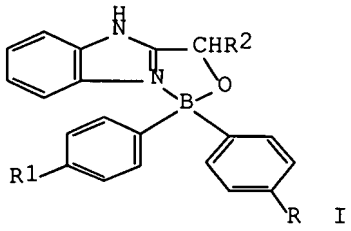
RN 137001-20-8 CAPLUS
CN Boron, bis(4-methoxyphenyl)(2-methyl-8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)



RN 137001-21-9 CAPLUS
CN Boron, bis(4-methoxyphenyl)(8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)


N
O
3+
B
C
OMe
C
OMe

L16 ANSWER 18 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:454817 CAPLUS Full-text
DOCUMENT NUMBER: 109:54817
TITLE: Boron compounds. (XIX). New organyloxydiarylborane chelates containing the virucide 2-(α-hydroxyalkyl)benzimidazole as ligands
AUTHOR(S): Yuan, Guozheng; Li, Guiying; Zhang, Guomin
CORPORATE SOURCE: Dep. Chem., Wuhan Univ., Guomin, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1987), 8(5), 398-402
CODEN: KTHPDM; ISSN: 0251-0790
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



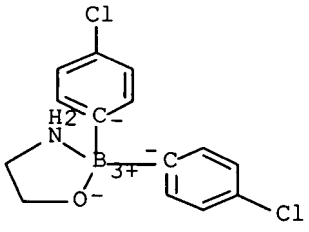
I

AB Title compds. I (R, R1 = H, Me, Cl; R2 = H, Ph) were prepared through the reaction of 2-(α-hydroxymethyl)benzimidazole or 2-(α- hydroxybenzyl)-benzimidazole with diarylborinic acid. These compds. were identified by elemental anal., MS, IR and UV spectroscopies.

IT ***61731-73-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 61731-73-5 CAPLUS

CN Boron, [2-(amino-κN)ethanolato-κO]bis(4-chlorophenyl)-, (T-4)-(9CI) (CA INDEX NAME)

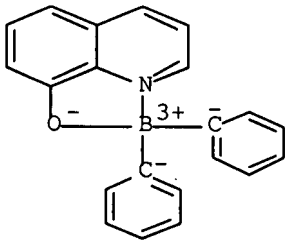


L16 ANSWER 17 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:143497 CAPLUS Full-text
DOCUMENT NUMBER: 114:143497
TITLE: Proton and boron-11 NMR spectroscopy of diarylboron chelates containing boron-nitrogen coordinate bonds and of triboranes
AUTHOR(S): Yu, Dingzhang; Yuan, Guozheng; Zhang, Gumin
CORPORATE SOURCE: Dep. Anal. Test. Sci., Wuhan Univ., Wuhan, Peop. Rep. China
SOURCE: Fenxi Ceshi Tongbao (1990), 9(4), 5-10
CODEN: FCTOE8; ISSN: 1000-3800
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

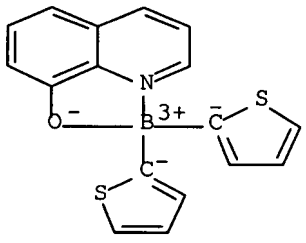
AB Spectroscopic characteristics of 1H FT-NMR and FT-IR of 25 diarylboron chelates with 8-hydroxyquinoline, benzimidazole, ethanolamine or amino acids were reported. 11B FT-NMR spectroscopy of Me4N+ B3H8- was described.

IT ***29190-60-1 74344-31-3 132722-11-3 132722-17-9***
RL: PRP (Properties)
(IR and NMR spectra of)

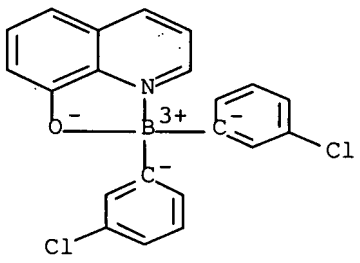
RN 29190-60-1 CAPLUS
CN Boron, diphenyl(8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)



RN 74344-31-3 CAPLUS
CN Boron, (8-quinolinolato-κN1,κO8)di-2-thienyl-, (T-4)- (9CI) (CA INDEX NAME)

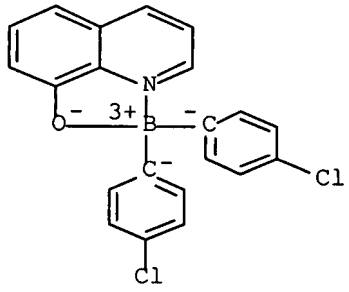


RN 132722-11-3 CAPLUS
CN Boron, bis(3-chlorophenyl)(8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)



RN 132722-17-9 CAPLUS

CN Boron, bis(4-chlorophenyl)(8-quinolinolato-κN1,κO8)-, (T-4)-(9CI) (CA INDEX NAME)



L16 ANSWER 26 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:528040 CAPLUS Full-text
DOCUMENT NUMBER: 81:128040
TITLE: Crystal and molecular structure of B,B-bis(p-fluorophenyl)boroxazolidine, (p-FC6H4)2BO(CH2)2NH2
AUTHOR(S): Rettig, Steven J.; Trotter, James
CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, Can.
SOURCE: Acta Crystallographica, Section B: Structural Crystallography and Crystal Chemistry (1974), B30, Pt. 9, 2139-45
CODEN: ACBCAR; ISSN: 0567-7408
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. Crystals of the title compound are orthorhombic with lattice parameters a 13.442(4), b 10.214(3), c 9.283(2) Å, Z = 4, space group P212121. The structure was solved by direct methods, and refined by electron-d. and full-matrix least-squares procedures to R = 0.047 for 1234 reflections. The 5-membered borox-azolidine ring is in a distorted half-chair conformation. Bond angles in the ring range from 99.9(2)° for OBN to 108.2(2)° for BOC. Bond lengths are: mean B-C 1.618(3), B-N 1.652(4), B-O 1.471(4), C-N 1.491(4), C-O 1.418(4), mean C-F 1.371(4), mean C-C(aromatic) 1.390(13), and C(sp3)-C(sp3) 1.494(6) Å. The structure consists of discrete mols. each linked to 6 others by an extensive network of O...H-N(O...N = 2.941(3) Å, F...H-N-(F...N = 3.171(4) Å, and F...H-C(F...C = 3.318(5) Å) hydrogen bonds.

IT ***25610-36-0***
RL: PRP (Properties)
(crystal structure of)

RN 25610-36-0 CAPLUS

CN Boron, [2-(amino-κN)ethanolato-κO]bis(4-fluorophenyl)-, (T-4)- (9CI) (CA INDEX NAME)